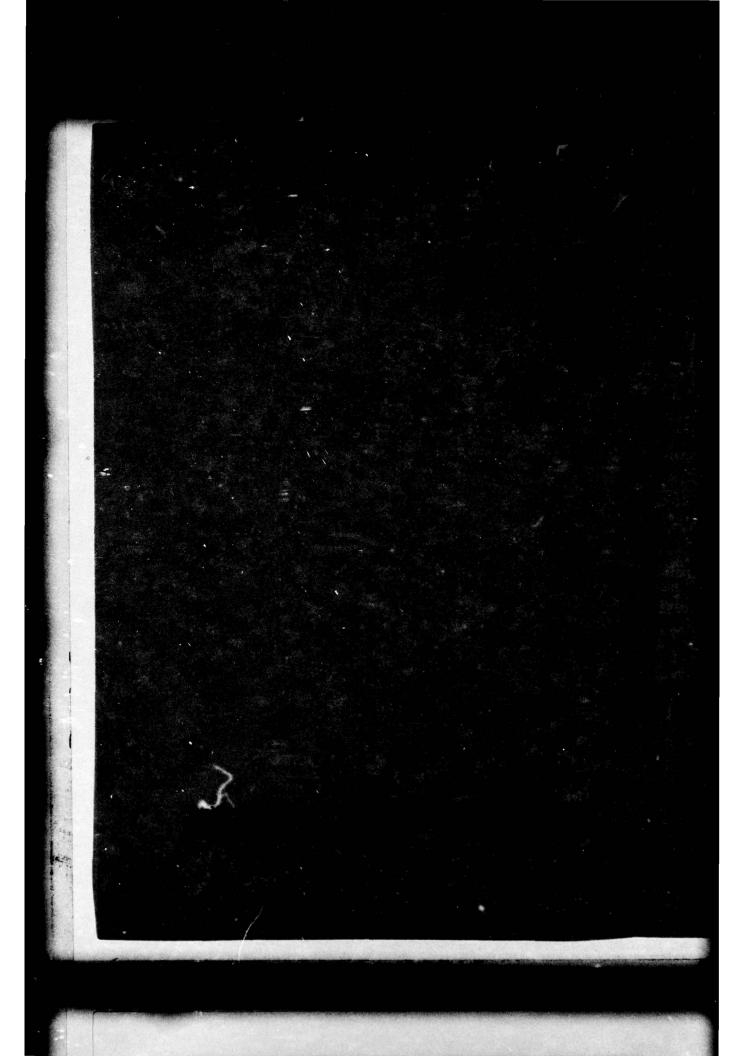


ADAU34042



Data Analysis.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report is presented to give a description of the mathematical and numerical analysis effort in support of the Air Force scientists engaged in basic research in the environmental sciences.

The scope of problems reported both in the particular discipline supported and the type of support is quite broad. Typically, the analysis involved: mathematical modelling, digital filtering, continuation of block #20. - Abstract

DD 1 JAN 73 1473

EDITION OF 1 NOV 65 IS OBSOLETE

Unclassified

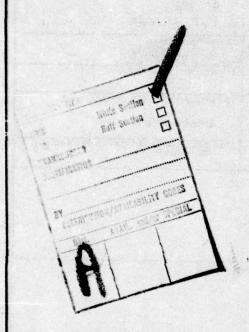
SECURITY CLASSIFICATION OF THIS PAGE (When Date Entered,

409 955

SECURITY CLASSIFICATION OF THIS PAGE(When Date Entered)

integral evaluations, solving systems of differential equations (both ordinary and partial), data fitting, and Fourier analysis. Application computer programs were also developed to not only check the analysis but also to produce data required by the scientists.

The duration of support is just as varied and lasted anywhere from a few days to many months. Therefore, some of the problems reported upon are analyzed, while others reached various degrees of evolution toward a complete final resolution.



LIST OF AUTHORS

Thomas M. Costello
Richard W. Doherty
Isaac Fried
Barry Hass
Paul E. Meehan
Joseph P. Noonan
Joseph F. Russell, Jr.
Marcel Schneeberger
Brendan J. Welch

FOREWORD

This support analysis and scientific programming was performed under contract to the Analysis and Simulation Branch (SUA) of the Air Force Geophysics Laboratory (AFGL), Hanscom Air Force Base, Massachusetts. Programs described herein and documentation of such can be obtained from the computer library of SUA.

PRECIDING PARTY

TABLE OF CONTENTS

	Page
LIST OF AUTHORS	iii
FOREWORD	v
TABLE OF CONTENTS	vii
Sharp Cutoff Non-Recursive Filter Design	1
Analysis of Electric Fields in Visual Aurora	3
Net Space-Charge-Limited Current Flow	9
Electron Capture From Tl ⁺ and Li ⁺	11
Study of a Dielectric Slab in a Waveguide	20
Analysis of a Waveguide Junction	23
Rocket Exhaust Plume Study	25
Interpretations of Spectroscopic Data	27
Study of Variational Principles in Approximations of Molecular Characteristics	28
Radio Antenna Program Conversion	30
Model for the Refractive Index of Stratospheric Aerosols	31
Phase Derived Navigation	33
Withdrawal Weighting Synthesis	36
Measurement of Ambient Electric Field	38
Contour of Earth Deformation Due to Chemical Explosion	40
Lamb Wave Velocity Dispersion	41
Acoustic Wave Beamshaping	43
A Calculation of Fourier Harmonics	44
Integral Computations Using Gauss-Mehler Quadrature	45
Computer Modification Used in the Calculation of Radial and Tangential Displacements of the Elastodynamic Field	48
Tape Evaluation	51
Potential Between Two Rare Gas Atoms	52
Numerical Mapping of Ionospheric Parameters on a Global Basis	55

TABLE OF CONTENTS (Cont.)

	Page
Tape Reformatting	56
Inversion of LIMB Airglow Measurements	57
Collimator Program Conversion	61
Signal Analysis of Rocket Data	62
Wavelength Peak Study	64
Statistical Analysis of Gas Measurement Data	65
ACKNOWLEDGEMENTS	66

SHARP CUTOFF NON-RECURSIVE FILTER DESIGN

Initiator : A. Slobodník, Jr.

Problem No.: 3057 Project No.: 5635

The purpose of this project is to design a sharp cutoff, flat top, bandpass filters using a Lagrange interpolation design algorithm. Several articles on this subject were gathered and read. Possible computationally efficient interpolation schemes were examined.

The technique to be investigated initially uses trigonometric polynomial approximation. Given desired values for

N = order of polynomial

Np = maximum number of passband ripples

Sp = maximum deviation allowable in the passb

Ss = maximum deviation allowable in the stopband.

The design algorithm first estimates an initial set of extremum frequencies $F_k^{(0)}$, $K=1,\ldots,N+1$, at which the extrema of the desired frequency response $H_0(F)$ are to be located. It then uses the barycenter form of the Lagrange interpolation formula to obtain an $N^{\underline{th}}$ order polynomial that passes through the maximum ripple values (1+Sp) in the passband and +Ss in the stopband) at these prescribed frequencies. In general, this first Lagrange polynomial will achieve its extrema at frequencies distinct from the estimated set of original frequencies $F^{(0)}$ and additional stages of the algorithm will be required.

The final algorithm is a slight extension of an algorithm due to Parks and McClellan. Basically, a weighted Chebyshev filter with trigonometric cosine polynomials is found for the step function,

H(f) = 1, $0 \le f \le FP$ H(f) = 0, $FP + DELF \le f \le 1/2$,

where DELF < 0 is introduced by the algorithm and adjusted iteratively until the Rs, RB tolerances are satisfied. Excellent results have been obtained with this approach.

The results were submitted to the investigators.

ANALYSIS OF ELECTRIC FIELDS IN VISUAL AURORA

Initiator : M. Smiddy.

Problem No.: 4535

Project No.: 8617

This problem deals with the determination of the ambient electric field vector as measured during a series of rocket flights into a visual aurora.

In the geomagnetic polar region, where the earth's magnetic field (carrying trapped radiation belt particles) dips into the atmosphere, plasma theory dictates that an electric field should be created. The electric fields should be very weak – a few tens of millivolts per meter.

The low values of the electric fields make measurements difficult and the exact locations of the field themselves are uncertain. Visible auroras, however, give clues as to where to look for them.

A Black Brant VC rocket was launched on April 4, 1972 into a visible aurora display over Fort Churchill, Canada.

Detection of the fields were made by six solid spheres mounted on three pairs of diametrically opposed booms. The spheres reach their respective local plasma potential, due to the high plasma conductivity. The potential difference between any sensor pair gives the electric field component along the boom direction. A spin was imparted to the vehicle about its longitudinal axis to enable the electric field to be measured anywhere in a direction normal to this axis. Due to the slow precession of the longitudinal vehicle axis itself the plane in which the electric field is sampled changes in space.

Each pair of booms will be analyzed separately. The first stage of the analysis consist in processing and merging the magnetic tapes containing the

attitude data of the rocket and the booms, and the tapes containing the values for the potential differences for each sensor pair. These merged tapes represent the input to the program written to analyze the ambient magnetic field.

Following is a functional description of the computer program written to analyze the data and a description of the mathematical method used.

The ambient electric field \vec{E}_A exists in space as a function of position and time, $\vec{E}_A = \vec{E}_A(\vec{r},t)$. Probes mounted on booms extending from a rocket measure a potential difference ΔV , when flying through regions of the ionosphere in which an electric field \vec{E} exists. If the probes are aligned along an axis $\vec{R}(t)$, moving with velocity $\vec{v}(t)$, through the earth's magnetic field $\vec{B}(\vec{r})$, then the total voltage measured is

$$\Delta V = \vec{E} \cdot \vec{R} = \vec{E}_{A} \cdot \vec{R} + \vec{v} \times \vec{B} \cdot \vec{R} \ .$$

The object of the program is to reconstruct \vec{E}_A from the experimental data consisting of ΔV , $\vec{R}/|R|$, \vec{v} , and \vec{B} , all versus time. \vec{v} and \vec{B} are obtained analytically.

The components E_x , E_y , and E_z of the ambient electric field can be approximated from

$$\vec{E}_A \cdot \vec{R} = \Delta V - \vec{v} \times \vec{B} \cdot \vec{R}$$

and the direction cosine of $\vec{R}(t)$ by fitting in the least-square sense to a polynomial of arbitrary degree n. The fitted field \vec{E}_A can be output as a list of the components vs. time or in form of Calcomp plots of the components vs. time.

The program is extensively documented and is logically broken down into the following parts:

- I. Initialization phase. Reads various parameters and initializes for each run.
- II. Read R data. Reads attitude data from tape and sets up the array of time points.
- III. Read E data.
- IV. Least-square analysis. Perform the least-square analysis.
- V. Output phase. Sets up printed output and writes required plots on plotter tape.

The electric field E(t) is defined as

$$\vec{E}(t) = \sum_{i=1}^{3} E_i(t) \vec{\mu}_i \qquad (\{\vec{\mu}_i\} \text{ o.n. basis of } \vec{R}) .$$

The object is to determine the components $E_i(t)$ given

$$y = \vec{E} \cdot \vec{R}$$
 and $\vec{R}(t)$.

We approximate E; (t) by a polynomial in t

$$\vec{E}_{i}(t) = \sum_{k=0}^{p_{i}} E_{ik} t^{k} . \qquad (1)$$

Define

$$S = \sum_{j=1}^{N} \left[\sum_{i=1}^{3} R_i(t_j) E_i t_j - y(t_j) \right]^2$$

by (1)

$$S = \sum_{k=1}^{N} \left[\left(\sum_{i=1}^{3} R_{i}(t_{j}) \sum_{k=0}^{p_{i}} E_{ik} t_{j}^{k} \right) - y(t_{j}) \right]^{2} ,$$

where N = Number of time points. Then calculate

$$\frac{\partial S}{\partial E_{\alpha\beta}} = 0 \quad \text{(least squares)}$$

which will produce $M = \sum_{i=1}^{3} (P_i + 1)$, equations

$$\begin{split} \frac{\partial S}{\partial E_{\alpha\beta}} &= \frac{\partial}{\partial E_{\alpha\beta}} \left(\sum_{j=1}^{N} \left[\left(\sum_{i=1}^{3} R_{i}(t_{j}) \sum_{k=0}^{p_{i}} E_{ik} t_{j}^{k} \right) - y(t_{j}) \right]^{2} \right) \\ &= 2 \sum_{j=1}^{N} \left[\sum_{i=1}^{3} R_{i}(t_{j}) \sum_{k=0}^{p_{i}} E_{ik} t_{j}^{k} - y(t_{j}) \right] \frac{\partial}{\partial E_{\alpha\beta}} \\ &= 2 \sum_{j=1}^{N} \left[\sum_{i=1}^{3} R_{i}(t_{j}) \sum_{k=0}^{p_{i}} E_{ik} t_{j}^{k} - y(t_{j}) \right] P_{\alpha}(t_{j})(t_{j})^{\beta} , \\ &= 2 \sum_{j=1}^{N} \left[\sum_{i=1}^{3} R_{i}(t_{j}) \sum_{k=0}^{p_{i}} E_{ik} t_{j}^{k} - y(t_{j}) \right] P_{\alpha}(t_{j})(t_{j})^{\beta} , \end{split}$$

setting $\partial S/\partial E_{\alpha\beta} = 0$ gives M equations

$$\sum_{j=1}^{N} \left[\sum_{i=1}^{3} \mathrm{R}_{i}(t_{j}) \sum_{k=0}^{p_{j}} \mathrm{E}_{ik} \; t_{j}^{k} \; \mathrm{R}_{\alpha}(t_{j}) \; t^{\beta} \right] = \sum_{j=1}^{N} y(t_{j}) \; \mathrm{R}_{\alpha}(t_{j}) \; t^{\beta}_{j} \; \; .$$

The coefficient of Eik is

$$\sum_{i=1}^N R_i(t_j) \ t_j^k \ R_{\alpha}(t_j) \ t_j^{\beta} \ . \label{eq:reconstruction}$$

These coefficients are the elements of an $M \times M$ matrix which together with the M right-hand sides form a system of M linear equations. This system is solved for the M unknowns E_{ik} by the method of matrix inversion. The SSP routine MINV is used to achieve this.

The rocket involved was spinning around its axis at a much faster rate than expected and this made it practically impossible to extract useful data for the intended analysis. It was, therefore, decided by the investigator to terminate the effort and analyze another rocket flight, reported under Problem No. 4764.

SPHERICAL ELECTROSTATIC ANALYZER (ELECTRONS) Black Brant VC A18,109-1 Payload EFIELD SPINNING NOSE TIP E FIELD ELECTRONICS SEA ELECTRONICS 3 AXIS DIGITAL DETECTORS PHOTOMETERS > SPARP CAL ELECTROSTATIC ANAL (7FP POSITIVE SONS) E F.ELD SENSORS 10 BIT PCM ENCODERS

NET SPACE-CHARGE-LIMITED CURRENT FLOW

Initiator : P. Gianino.

Problem No.: 4630 Project No.: 5621

This problem is aimed at solving nonlinear Volterra integral equations of the first and second kind, numerically, for the net space-charge-limited current flowing between 2 plane-parallel plates emitting secondary electrons. These electrons are emitted when radiation impinges in the metal plates.

The problem consists of 5 parts: (a) compute an upper threshold, (b) compute a lower threshold, (c) compute a threshold for 20-40 points between the upper and lower threshold (the space-charge-limited region), (d) and (e) evaluate some expressions which depend on the answers obtained in (a) and (b).

A typical integral that occurs in (a), (b), and (c) is of the form

$$D^{2} = \frac{1}{415} \int_{0}^{.402 \text{VE}} \frac{du}{\sqrt{h^{+}(u) + \text{Le}^{-.402 \text{VE}} h^{-}(u)}},$$

where $h^{\pm}(u) = e^{u} - 1 \pm 2\sqrt{u/\pi} + e^{u}$ erf \sqrt{u} , L and D are parameters with known values. The problem is to find the value of VE for which equality holds, i.e., VE is the desired threshold.

There are several problems which must be overcome before the problem can be solved:

- (1) the integrand has a singularity at u = 0;
- (2) the problem is highly nonlinear;

- (3) each change in VE changes the integrand;
- (4) the expression e^{u} erf \sqrt{u} in $h^{\pm}(u)$ creates substantial numerical problems.
- (2) and (3) are surmountable since the integrand and the integral are both monotonic functions of VE. This allows a use of some well-known iterative techniques.
- (1) was overcome after a substantial study of the sensitivity of values of the integral to changes in the lower limit (i.e., replacing 0 by ϵ and finding an ϵ suitable for the purposes of this study).
- (4) was the most difficult to get around. A number of published formulae were used with little success. A continued fraction expansion for e^{X^2} erf X was coded and discovered to be wrong for X \ll 1. Finally, a combination of published and unpublished results was coded and incorporated successfully into the program.

In solving parts (1) and (2), the problem was treated in two parts:

- (a) Find 2 values of VE for which the right-hand side was greater and less than the desired value, D^2 .
- (b) Apply the technique of "interval halving" to the interval found in (a), to obtain the solution VE.

A similar approach was used in (c). All integrations were performed by using a 32 point Gauss-quadrature.

The problem was completed and the results given to the investigator.

ELECTRON CAPTURE FROM TI+ AND LI+

Initiator : R. Mapleton

Problem No.: 4666 Project No.: 8627

THE PHYSICAL PROBLEM

This problem is concerned with estimating the cross section for the reaction

$$H^+ + TI^+(6S^2: {}^1S) \longrightarrow \sum_n H(n) + \sum_m TI^{++}(m)$$
 (1)

for energies in the range $1 \le E \le 16$ keV, where n denotes the states of atomic hydrogen and m denotes the states of the doubly-ionized Thallium atom Tl^{++} . Since capture into H(1S) dominates, we can write Σ_n H(n) = H(1S) in (1); also, since for these impact energies, cross section for capture of the outermost electron dominates, we can simplify (1) to obtain

$$H^+ + Tl^+ (6S^2: ^1S) \longrightarrow H(1S) + Tl^{++} (6S: ^2S)$$
 (2)

using, respectively, 1 electron and 2 electron ions for Tl+ and Tl++.

We next construct a Schrodinger wave equation for (2). For the impact version of this problem, the equation, in atomic units, is

$$\left(H-i\frac{\partial}{\partial t}\right)\psi=0, \qquad (3)$$

where H denotes the Hamiltonians. After capture, the Hamiltonian is given by

H = H(p1) + H(C⁺⁺2) -
$$\frac{1}{r_{2p}}$$
 + $\frac{1}{r_{12}}$ + $\frac{V_f(C^{++}1)}{2}$ (4)

and initially (before capture) the Hamiltonian H is given by

$$H = H(C^{+}12) - \frac{1}{r_{2p}} - \frac{1}{r_{1p}} , \qquad (5)$$

where H is the Hamiltonian for the hydrogen atom, the Tl^{++} (6S), the doubly-ionized Thallium atom and Tl^{++} (6S²), the singly-ionized Thallium atom. Also, in (5), p denotes proton, subscript 1 denotes electron 1, subscript 2 denotes electron 2, C^{++} denotes the Tl^{++} core and C^{+} the Tl^{+} core. Distances between particles are denoted by r_{12} , r_{p1} , r_{p2} , r_{1n} , and r_{2n} with n denoting the Tl nucleus.

The Hamiltonians in (4) are given by

$$H(p1) = -\frac{1}{2} \nabla_{p1} - \frac{1}{r_{p1}}$$
 (6)

and

$$H(C^{++}2) = -\frac{1}{2}\nabla_{2n} + \frac{V_f(C^{++}2)}{2}$$
, (7)

where [V_s(C⁺⁺2)]/2 is derived from the eigen equation

$$H(C^{++}2) \psi(TI^{++}) = -\epsilon(++) \psi(TI^{++})$$
 (8)

We now change coordinates, from the hydrogen atom to the Tl^+ electron coordinates \underline{r}_{1n} , \underline{r}_{2n} and obtain from (4):

$$H = \left(-\frac{1}{2}\nabla_{n1}^{2} - \frac{1}{2}\nabla_{n2}^{2} + \frac{V_{f}(C^{++1})}{2} + \frac{V_{f}(C^{++2})}{2} + \frac{1}{r_{12}}\right) - \frac{1}{r_{1p}} - \frac{1}{r_{2p}}$$

$$\underline{r}_{pj} = \underline{r}_{nj} - \underline{R}$$

$$\underline{r}_{12} = \underline{r}_{n1} - \underline{r}_{n2}$$

$$(10)$$

Apart from the Coulomb interactions, (9) represents the Hamiltonian for the function $\Phi^2(TT^{+}6S)$. Replacing $V_f(C^{+}j)$ by $V_i(C^{+}j) - (1/r_{12})$ in (9), we have

$$H = \left(-\frac{1}{2}\nabla_{\mathbf{n}1}^{2} - \frac{1}{2}\nabla_{\mathbf{n}2}^{2} + \frac{V_{\mathbf{i}}(C^{+1})}{2} + \frac{V_{\mathbf{i}}(C^{+2})}{2} - \frac{1}{r_{12}}\right) - \frac{1}{r_{1p}} - \frac{1}{r_{2p}} \quad (11)$$

$$= H_{1} - \frac{1}{r_{1p}} - \frac{1}{r_{2p}} \tag{12}$$

and we approximate H, by

$$H_{s} \psi(TI^{+}) = -\epsilon(+) \psi(TI^{+})$$
, (13)

where $\epsilon(+)$ denotes the (experimental) energy of Tl^+ . Next, the assumption is made that the interaction of $\mathrm{e}(H)$ with the Tl^{++} ion is represented by $\mathrm{V_i}(\mathrm{C}^+\mathrm{1})$, imagining $\mathrm{Tl}^+(6\mathrm{S}^2)$ as constructed of $\mathrm{Tl}^{++}(6\mathrm{S})$ and $\mathrm{e}(H)$, we get

$$\frac{V_{f}(C^{++}j)}{2} = \frac{V_{f}(C^{+}j)}{2} - \frac{1}{r_{12}}, \qquad j = 1, 2, \qquad (14)$$

which can be seen to be exact at large distances from the nucleus.

We now consider the scattering problem: Let

$$\Psi = A(t) \psi_t + B(t) \psi_t , \qquad (15)$$

where ψ_i and ψ_f represent the wave functions of the system before and after scattering, respectively. These are given by

$$\psi_{i} = \chi(\underline{\mathbf{r}}_{1n}, \underline{\mathbf{r}}_{2n}) \exp \left\{ i \left[\left(-\epsilon - \frac{\mathbf{v}^{2}}{2} \right) \mathbf{t} - \frac{\mathbf{v}}{2} \left(\underline{\mathbf{s}}_{1} + \underline{\mathbf{s}}_{2} \right) \right] \right\}$$
 (16)

and

$$\psi_{\mathbf{f}} = \chi(\underline{\mathbf{r}}_{\mathbf{p}1}, \underline{\mathbf{r}}_{\mathbf{2n}}) \exp \left\{ i \left[\left(\epsilon_1 + \mu - \frac{\mathbf{v}^2}{4} \right) \mathbf{t} + \frac{\underline{\mathbf{v}}}{2} \left(\underline{\mathbf{s}}_1 - \underline{\mathbf{s}}_2 \right) \right] \right\} , (17)$$

where

$$\underline{s}_{i} = \underline{r}_{i} - \frac{\underline{r}_{p} + \underline{r}_{n}}{2} = \underline{r}_{nj} - \frac{\underline{R}}{2} = \underline{r}_{pj} + \frac{\underline{R}}{2}$$
, $\underline{R} = \underline{r}_{p} - \underline{r}_{n}$ (18)

and

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_i} + \mathbf{v} \cdot (\nabla_{\mathbf{n}1} + \nabla_{\mathbf{n}2}) = \frac{\partial}{\partial t_f} + \frac{\mathbf{v}}{2} \cdot (\nabla_{\mathbf{n}2} - \nabla_{\mathbf{1}p}) \quad . \tag{19}$$

Also,

$$\alpha_{i} = \epsilon - \frac{V^{2}}{2}$$

$$t = t_{i} = t_{f}$$

$$\beta_{f} = \epsilon_{1} + \mu_{f} - \frac{V^{2}}{4}$$

$$\gamma = (\alpha_{i} - \beta_{f}) t$$

$$(1) = -\epsilon \alpha(r_{i})$$

$$\left(-\frac{1}{2}\,\triangledown_{1\mathrm{p}}^2-\frac{1}{\mu_{1\mathrm{p}}}\right)\varphi(\mu_{1\mathrm{p}})=-\,\epsilon_1\varphi(\underline{\mathbf{r}}_{1\mathrm{p}})$$

$$\left(-\frac{1}{2}\nabla_{2n}^{2}+\frac{1}{2}\nabla_{f}(C^{++}2)\right)\psi(\underline{r}_{2n})=-\mu\psi(r_{2n})$$

and

$$H_{i}\chi(\underline{\mathbf{r}}_{1n},\underline{\mathbf{r}}_{2n}) = -\epsilon\chi(\underline{\mathbf{r}}_{1n},\underline{\mathbf{r}}_{2n}) \quad . \tag{20}$$

The scattering equations, from (3) are then given by

$$\left(\psi_{\mathbf{i}}, \left[H - i \frac{\partial}{\partial t}\right] \psi\right) = 0 \tag{21}$$

and

$$\left(\psi_{\mathbf{f}}, \left[\mathbf{H} - \mathbf{i} \frac{\partial}{\partial \mathbf{t}}\right] \psi\right) = 0 \quad . \tag{22}$$

From (11), we have

$$\left(-\frac{1}{2}\nabla_{1s}^{2} - \frac{1}{2}\nabla_{2s}^{2} - \frac{1}{r_{1p}} + \frac{V_{f}(C^{++}2)}{2} - i\frac{\partial}{\partial t}\right)\varphi_{f} = 0$$
 (23)

and similarly

$$\left(-\frac{1}{2}\nabla_{18}^{2} - \frac{1}{2}\nabla_{28}^{2} - \frac{1}{r_{12}} + \frac{V_{i}(C^{+1})}{2} + \frac{V_{i}(C^{+2})}{2} - i\frac{\partial}{\partial t}\right)\psi_{i} = 0 \quad . \quad (24)$$

Now, writing

 $\left(H - i \frac{\partial}{\partial t}\right) \psi_{i} = -v \psi_{i} \tag{25}$

and

$$\left(H - i\frac{\partial}{\partial t}\right)\psi_{f} = u\psi_{f} \tag{26}$$

we then can obtain, from (15) and using (18) - (24), the following coupled system of (complex) ordinary differential equations:

$$i(1 - |S|^{2}) \mathring{A}(t) = [V_{ii} - S*V_{fi}] A(t) + [U_{if} - S*U_{ff}] B(t)$$

$$i(1 - |S|^{2}) \mathring{B}(t) = [V_{fi} - SV_{ii}] A(t) + [U_{ff} - SU_{if}] B(t)$$
(27)

with the initial conditions

A
$$(t = -\infty) = 1$$

B $(t = -\infty) = 0$, (28)

where

$$U \approx -\left(\frac{1}{r_{1p}} + \frac{1}{r_{2p}}\right) \tag{29}$$

and

$$V \approx \frac{V_{i}(C^{+1})}{2} - \frac{1}{r_{12}} - \frac{1}{r_{2p}} + \frac{V_{i}(C^{+2})}{2} - \frac{V_{f}(C^{+2})}{2}$$

and we write

$$V_{ii} = \int_0^\infty \int_0^\infty \psi_i^* \, V \, \psi_i \, d\mathbf{r}_{1n} \, d\mathbf{r}_{2n}$$

$$V_{fi} = \int_0^\infty \int_0^\infty \psi_f^* \, V \, \psi_i \, d\mathbf{r}_{1n} \, d\mathbf{r}_{2n}$$
(Continued)

$$U_{if} = \int_0^\infty \int_0^\infty \psi_i^* U \psi_f dr_{1n} dr_{2n}$$

$$U_{ff} = \int_0^\infty \int_0^\infty \psi_f^* U \psi_f dr_{1n} dr_{2n}$$
and
$$S = \int_0^\infty \int_0^\infty \psi_f^* \psi_i dr_{1n} dr_{2n} .$$
(30)

Thus, to obtain the quantity of interest, the cross section for capture from ${\rm Tl}^+(6{\rm S}^2)$ into ${\rm H(1S)}$ + ${\rm Tl}^{++}(6{\rm s})$ by protons, we have to evaluate

$$Q = 4\pi \rho_0^2 \int_0^\infty \rho |B| (t = \infty) |^2 d\rho , \qquad (31)$$

where $R^2 = \rho^2 + v^2t^2$, $v = 0.2\sqrt{E}$ and t is time, ρ is the impact parameter, and v is the initial velocity with respect to the Tl^+ ion at rest and E is the energy. This, in turn, requires the solution of the initial value problem, given by (27), (28) for sufficient values of the impact parameter ρ to enable the integration in (31) to be carried out. Note that, in turn, the solution of (27), (28) is in itself extremely difficult due to the complexity of the elements of the coefficient matrix, given by (30). Thus, to make the problem at all numerically tractable, a number of simplifications must be imposed.

First, since the radial wave functions for Tl^+ and Tl^{++} and the interactions $V_i(C^+j)$ and $V_f(C^{++}j)$, j=1,2 are given in numerical form, it is not possible to simplify the matrix elements. However, if momentum transfer is neglected (i.e., set to zero) then we can obtain the simplification given by omitting the factors $\exp[(-i/2) \underline{v}(\underline{S}_1 + \underline{S}_2)]$ and $\exp[(-i/2) \underline{v}(\underline{S}_1 - \underline{S}_2)]$ from the expressions for ψ_i and ψ_f , respectively, in (16) and (17), yielding

and
$$\psi_{\mathbf{i}} = \chi(\underline{\mathbf{r}}_{1\mathbf{n}}, \underline{\mathbf{r}}_{2\mathbf{n}}) \exp \left[i\left(\epsilon - \frac{\mathbf{v}^2}{2}\right)^{\frac{1}{2}}\right]$$

$$\psi_{\mathbf{f}} = \chi(\underline{\mathbf{r}}_{\mathbf{p}1}, \underline{\mathbf{r}}_{\mathbf{p}2}) \exp \left[i\left(\epsilon_1 + \mu - \frac{\mathbf{v}^2}{4}\right)\mathbf{t}\right].$$
(32)

Next, since the integrals in (30) are effectively double integrals, we will expand the integrands in Legendre series, using

$$\mathbf{r}_{\mathbf{p}\mathbf{j}} = \mathbf{r}_{\mathbf{n}\mathbf{j}} - \mathbf{R} \tag{33}$$

with $R^2 = \rho^2 + v^2t^2$, etc. The independent variables (r_{1n}, r_{2n}, t) are used since the wave functions are given numerically in these variables. The Legendre's expansions used are

$$|\mathbf{r}_{nj} - \mathbf{R}|^{-1} = \frac{1}{r>}$$

$$|\mathbf{r}_{n1} - \mathbf{r}_{n2}|^{-1} = \frac{1}{\mathbf{r}_{nj}>}$$

$$\frac{\exp(-|\mathbf{r}_{n1} - \mathbf{R}|)}{|\mathbf{r}_{n1} - \mathbf{R}|} = \frac{1}{2\mathbf{r}_{n1}\mathbf{R}} (e^{\mathbf{r}<} - e^{-\mathbf{r}<}) e^{-\mathbf{r}>}$$

$$\exp(-|\mathbf{r}_{1n} - \mathbf{R}|) = \frac{e^{\mathbf{r}<} - e^{-\mathbf{r}<}}{2\mathbf{r}<} \left(1 + \frac{1}{r>}\right) - \left(\frac{e^{-\mathbf{r}<} + e^{-\mathbf{r}<}}{r>}\right) e^{-\mathbf{r}>},$$
(34)

where < and > denote, respectively, the lesser and greater of the two variables on the left-hand side. The functions $P(Tl^{+})$, $\psi(Tl^{++})$ correspond to rR(r), where R(r) is the corresponding radial function. Also, the functions P and ψ are normalized, i.e.,

$$\int_0^\infty |P^2(x)| dx = \int_0^\infty |\psi^2(x)| dx = 1 , \qquad (35)$$

and, as well as the interactions Vi, are given numerically. Then, using (34) in (30), the matrix elements become

$$S = \int_0^\infty \psi(x) \ P(x) \left\{ \int_R^\infty y \left(\left[\frac{e^R - e^{-R}}{R} \right] \left(1 + \frac{1}{y} \right) - \frac{e^R + e^{-R}}{y} \right) P(y) \ e^{-y} \ dy \right.$$

$$+ e^{-R} \int_0^R y \left(\frac{e^y - e^{-y}}{y} \left(1 + \frac{1}{R} \right) - \frac{e^y + e^{-y}}{R} \right) P(y) \ dy \right\} dx \quad . \quad (36)$$

$$\begin{split} &V_{11} = -2 \Biggl(\int_{R}^{\infty} \frac{p^{2}(x)}{x} \, dx + \frac{1}{R} \int_{0}^{R} P^{2}(x) \, dx \Biggr) \; . \end{aligned} \tag{37} \\ &V_{f1} = -S_{1}(R) \Biggl\{ \int_{R}^{\infty} \frac{\psi(x) P(x)}{x} \, dx + \frac{1}{R} \int_{0}^{R} \psi(x) P(x) \, dx \Biggr\} \\ &- \Biggl\{ \frac{e^{R} - e^{-R}}{R} \int_{R}^{\infty} P(x) \, e^{-x} \, dx \\ &+ \frac{e^{-R}}{R} \int_{0}^{R} \left[e^{x} - e^{-x} \right] P(x) \, dx \Biggr\} \int_{0}^{\infty} \psi(y) P(y) \, dy \; . \end{aligned} \tag{38} \\ &U_{1f} = \Biggl\{ \int_{R}^{\infty} P(x) \, x \Biggl[\frac{e^{R} - e^{-R}}{R} \Biggl(1 + \frac{1}{x} \Biggr) - \frac{e^{R} + e^{-R}}{x} \Biggr] e^{-x} \\ &+ e^{-R} \int_{0}^{R} P(x) \, x \Biggl[\frac{e^{x} - e^{-x}}{x} \Biggl(1 + \frac{1}{R} \Biggr) - \frac{e^{x} + e^{-x}}{R} \Biggr] \Biggr\} \\ &\times \Biggl\{ \frac{V_{1}(C^{+}x)}{2x} \int_{0}^{\infty} P(y) \, \psi(y) \, dy - \int_{x}^{\infty} P(y) \, \psi(y) \, dy - \frac{1}{x} \int_{0}^{x} P(y) \, \psi(y) \, dy \Biggr\} \\ &- \int_{R}^{\infty} \frac{P(y) \, \psi(y)}{y} \, dy - \frac{1}{R} \int_{0}^{R} P(y) \, \psi(y) \, dy \Biggr\} \, dx \; . \end{aligned} \tag{39} \\ &U_{ff} = \frac{1}{2} \Biggl\{ \int_{R}^{\infty} x^{2} \Biggl[\frac{e^{2R} - e^{-2R}}{R} \Biggl(2 + \frac{1}{x} \Biggr) - 2 \Biggl(\frac{e^{2R} + e^{-2R}}{R} \Biggr) \Biggr] e^{-2x} \\ &+ e^{-2R} \int_{0}^{R} x^{2} \Biggl[\frac{e^{2x} - e^{-2x}}{x} \Biggl(2 + \frac{1}{R} \Biggr) - 2 \Biggl(\frac{e^{2x} + e^{-2x}}{R} \Biggr) \Biggr] \Biggr\} \\ &\times \Biggl\{ \frac{V_{1}(C^{+}x)}{2x} - \int_{x}^{\infty} \frac{\psi^{2}(y)}{y} \, dy - \frac{1}{x} \int_{0}^{x} \psi^{2}(y) \, dy \end{aligned} \tag{Continued}$$

$$-\int_{R}^{\infty} \frac{\psi^{2}(y)}{y} dy - \frac{1}{R} \int_{0}^{R} \psi^{2}(y) dy dy dx , \qquad (40)$$

where x and y are dummy variables of integration.

We next separate A and B into the real and complex parts with the result that we now have, a coupled system of four ordinary (real) differential equations in four unknowns. We have

$$A = C + D_{i}$$
, $B = E + F_{i}$, (41)

hence, (27) and (28) become the initial value problem

$$(1 - |S|^{2}) \dot{C}(t) = I_{11}D(t) + I_{12}[-E(t) \sin \gamma + F(t) \cos \gamma]$$

$$-(1 - |S|^{2}) \dot{D}(t) = I_{11}C(t) + I_{12}[E(t) \cos \gamma + F(t) \sin \gamma]$$

$$(1 - |S|^{2}) \dot{E}(t) = I_{21}[C(t) \sin \gamma + D(t) \cos \gamma] + I_{22}F(t)$$

$$-(1 - |S|^{2}) \dot{F}(t) = I_{21}[C(t) \cos \gamma - D(t) \sin \gamma] + I_{22}E(t)$$

$$(42)$$

with initial conditions

$$C(-\infty) = 1$$
; $D(-\infty) = E(-\infty) = F(-\infty) = 0$. (43)

Note that the variable γ arises from (16) and (17) and is defined by (20), i.e.,

$$\gamma = \left(\epsilon - \frac{V^2}{2}\right)t \quad . \tag{44}$$

Also, that we have

$$I_{11} = -V_{ii} + SV_{fi} - SU_{if} + S^{2}U_{ff}$$

$$I_{12} = I_{21} = U_{fi} - SU_{ff}$$

$$I_{22} = U_{ff}$$

$$U_{fi} = U_{if}$$
(45)

with Vii, S, etc. given by (40).

Finally, note that it can be shown that

$$T(t) = |C(t)|^{2} + |D(t)|^{2} + |E(t)|^{2} + |F(t)|^{2} + 2S\{[C(t) E(t) + D(t) F(t)] \cos \gamma + [C(t) F(t) - D(t) E(t)] \sin \gamma\}$$

evaluated at $t = \infty$, is equal to

$$\int_0^\infty \psi^2(x) \ dx \ ,$$

i.e., at t=0, for the case of momentum transfer included, we have $T(\infty)=1$, hence, the closeness of the calculated value of T at $t=\infty$ to 1, indicates the correctness of the numerical solution, with the simplifications as detailed above.

Programs were developed to solve these equations and the results were presented to the investigator.

STUDY OF A DIELECTRIC SLAB IN A WAVEGUIDE

Initiator : H. Steyskal.

Problem No.: 4669
Project No.: 4600

This problem studies the mode propagation for a waveguide loaded with a dielectric slab.

A program was written which iteratively obtains a normalized complex wave number, $\beta_{\rm m}$, which is determined from the following equation

$$\beta_{\mathbf{m}}^{(\mathbf{n})} = \beta_{\mathbf{m}}^{(\mathbf{n}-1)} + \Delta \beta_{\mathbf{m}}^{(\mathbf{n}-1)}$$

for each mode m, where

m = 1, 2, ..., M as an outer index n = 1, 2, ..., N as an inner index ,

and where $\beta_{\mathbf{m}}^{(0)}$ is the complex conjugate of

$$\sqrt{k^2 - \left(\frac{m\pi}{2w}\right)^2}$$
.

If m = even number, then

$$\Delta\beta_{m}^{(n-1)} = \frac{-\delta B_{c}\left(p_{m}^{(n-1)}, q_{m}^{(n-1)}, b_{m}^{(n-1)}, c_{m}^{(n-1)}, c_{m}^{(n-1)}\right) - B\left(p_{m}^{(n-1)}, q_{m}^{(n-1)}, b_{m}^{(n-1)}, c_{m}^{(n-1)}\right)}{B_{\beta}\left(p_{m}^{(n-1)}, q_{m}^{(n-1)}, b_{m}^{(n-1)}, c_{m}^{(n-1)}, \beta_{m}^{(n-1)}\right)}$$

$$B = \cos (qc) \frac{\sin p(a+b)}{p} + \left[\frac{1}{q} \cos (pb) \cos (pa) - q \frac{\sin (pb)}{p} \frac{\sin (pa)}{p} \right] \sin (qc)$$

$$\begin{split} \mathbf{B}_{\mathbf{C}} &= (1-\epsilon) \frac{\mathbf{k}^2}{\mathbf{p}^2} \left[\cos \left(\mathbf{qc} \right) \sin \left(\mathbf{pa} \right) + \frac{\mathbf{p}}{\mathbf{q}} \sin \left(\mathbf{qc} \right) \cos \left(\mathbf{pa} \right) \right] \sin \left(\mathbf{pb} \right) \\ \mathbf{B}_{\boldsymbol{\beta}} &= \boldsymbol{\beta} \left\{ \left[\frac{\mathbf{a} + \mathbf{b} + \mathbf{c}}{\mathbf{p}^2} \sin \left(\mathbf{pa} \right) + \frac{1}{\mathbf{p}^3} \cos \left(\mathbf{pa} \right) \right] \sin \left(\mathbf{pb} \right) \right. \\ &+ \left. \left[\frac{1}{\mathbf{p}^3} \sin \left(\mathbf{pa} \right) - \left(\frac{\mathbf{a} + \mathbf{b}}{\mathbf{p}^2} + \frac{\mathbf{c}}{\mathbf{q}^2} \right) \cos \left(\mathbf{pa} \right) \right] \cos \left(\mathbf{pb} \right) \right\} \cos \left(\mathbf{qc} \right) \\ &+ \boldsymbol{\beta} \left\{ \left[\left(\frac{1}{\mathbf{p}^2 \mathbf{q}} - \frac{2\mathbf{q}}{\mathbf{p}^4} \right) \sin \left(\mathbf{pa} \right) + \left(\frac{\mathbf{b} + \mathbf{c}}{\mathbf{pq}} + \frac{\mathbf{aq}}{\mathbf{p}^3} \right) \cos \left(\mathbf{pa} \right) \right] \sin \left(\mathbf{pb} \right) \\ &+ \left[\left(\frac{\mathbf{a} + \mathbf{c}}{\mathbf{pq}} + \frac{\mathbf{bq}}{\mathbf{p}^3} \right) \sin \left(\mathbf{pa} \right) + \frac{1}{\mathbf{q}^3} \cos \left(\mathbf{pb} \right) \right] \right\} \sin \left(\mathbf{qc} \right) \ . \end{split}$$

If m = odd number, then

$$\begin{split} \Delta\beta_{\mathbf{m}}^{(n-1)} &= \frac{-\delta D_{\mathbf{c}} \left(p_{\mathbf{m}}^{(n-1)}, q_{\mathbf{m}}^{(n-1)}, b_{\mathbf{m}}^{(n-1)}, c_{\mathbf{m}}^{(n-1)}\right) - D \left(p_{\mathbf{m}}^{(n-1)}, q_{\mathbf{m}}^{(n-1)}, b_{\mathbf{m}}^{(n-1)}, c_{\mathbf{m}}^{(n-1)}\right)}{D_{\beta} \left(p_{\mathbf{m}}^{(n-1)}, q_{\mathbf{m}}^{(n-1)}, b_{\mathbf{m}}^{(n-1)}, c_{\mathbf{m}}^{(n-1)}, \beta_{\mathbf{m}}^{(n-1)}\right)} \\ D &= \cos \left(qc\right) \cos p(a+b) - \left[q \cos \left(pb\right) \frac{\sin \left(pa\right)}{p} + \frac{p}{q} \sin \left(pb\right) \cos \left(pa\right)\right] \sin \left(qc\right) \\ D_{\mathbf{c}} &= (1-\epsilon) \ k^2 \left[\cos \left(qc\right) \frac{\sin \left(pa\right)}{p} + \frac{\sin \left(qc\right)}{q} \cos \left(pa\right)\right] \cos \left(pb\right) \\ D_{\beta} &= \frac{\beta}{2} \left\{ \left[\frac{2a+2b+c}{p} + \frac{cp}{q^2}\right] \sin p(a+b) + \left[\frac{c}{p} - \frac{cp}{q^2}\right] \sin p(a-b)\right\} \cos \left(qc\right) \\ &+ \frac{\beta}{2} \left\{ \frac{-(p^2-q^2)^2}{p^3 q^3} \sin p(a+b) + \left[\frac{p}{q^3} - \frac{q}{p^3}\right] \sin p(a-b) + \left[\frac{a+b}{p} \left(\frac{q}{p} + \frac{p}{q}\right) + \frac{2c}{q}\right] \cos p(a+b) + \frac{a-b}{p} \left(\frac{q}{p} - \frac{p}{q}\right) \cos p(a-b)\right\} \sin \left(qc\right) \end{array}$$

If m = even or odd, then

$$\begin{aligned} \mathbf{p}_{\mathbf{m}}^{(n-1)} &= \sqrt{k^2 - \left(\beta_{\mathbf{m}}^{(n-1)}\right)^2} \\ \mathbf{q}_{\mathbf{m}}^{(n-1)} &= \mathrm{Re} \left\{ \sqrt{\epsilon k^2 - \left(\beta_{\mathbf{m}}^{(n-1)}\right)^2} \right\} \\ \mathbf{c}_{\mathbf{m}}^{(n-1)} &= (n-1) \ \delta \\ \mathbf{b}_{\mathbf{m}}^{(n-1)} &= \mathbf{w} - \mathbf{a} - \mathbf{c}_{\mathbf{m}}^{(n-1)} \end{aligned}.$$

Note that everywhere the following are complex numbers: p, β , $\Delta\beta$, D, D_c, D_β, B, B_c, B_β.

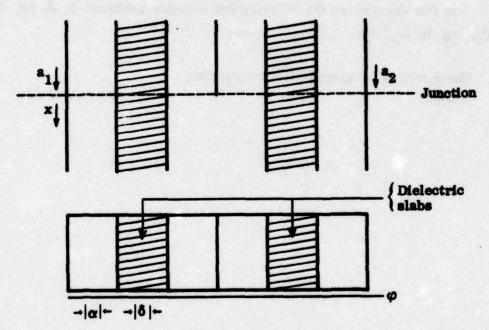
The results were given to the investigator,

ANALYSIS OF A WAVEGUIDE JUNCTION

Initiator : R. Mailloux

Problem No.: 4670
Project No.: 4600

The purpose of this problem is to produce a modal analysis of a waveguide junction. The program solves the problem of the junction of three waveguides. Each waveguide is partially loaded with dielectric as shown below.



The parameters M and N are related to the number of modes in the large waveguide and the small waveguides. Aplitudes a_1 and a_2 are the small waveguide excitation coefficients and ϵ is the relative dielectric constant of the dielectric slabs.

A system of N linear equations (corresponding to the N modes in the wave-guide) are solved.

$$\begin{pmatrix} \mathbf{2}^{\mathbf{K}_{2}} \\ \mathbf{0} \\ \vdots \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{C}_{11} & \cdots & \mathbf{C}_{N1} \\ \vdots & & \vdots \\ \mathbf{C}_{N,1} & \cdots & \mathbf{C}_{N,N} \end{pmatrix} \begin{pmatrix} \mathbf{V}_{1} \\ \mathbf{V}_{2} \\ \vdots \\ \mathbf{V}_{N} \end{pmatrix},$$

where the vector \vec{V} is solved, K_2 is an input parameter, the matrix C is a function of an array B, and

$$\begin{split} \mathbf{B_{mn}} &= \frac{\mathbf{A_{2m}A_{n}}}{\sqrt{2}} \, e^{-i \arg P_{2m}P_{n}} \, \left[\frac{\sin \left[\alpha (\mathbf{P_{2m} - P_{n}})\right]}{\mathbf{P_{2m} - P_{n}}} - \frac{\sin \left[\alpha (\mathbf{P_{2m} + P_{n}})\right]}{\mathbf{P_{2m} - P_{n}}} \right] \\ &+ \frac{\mathbf{D_{2m}D_{n}}}{\sqrt{2}} \, \left[\frac{\sin \left[(\mathbf{Q_{2m} - Q_{n}})(1 - \gamma) + \theta_{2m} - \theta_{n}\right] - \sin \left[\alpha (\mathbf{Q_{2m} - Q_{n}}) + \theta_{2m} - \theta_{n}\right]}{\mathbf{Q_{2m} - Q_{n}}} \right. \\ &- \frac{\sin \left[(\mathbf{Q_{2m} + Q_{n}})(1 + \gamma) + \theta_{2m} + \theta_{n}\right] - \sin \left[\alpha (\mathbf{Q_{2m} + Q_{n}}) + \theta_{2m} + \theta_{n}\right]}{\mathbf{Q_{2m} + Q_{n}}} \\ &+ \frac{\mathbf{C_{am}C_{n}}}{\sqrt{2}} \, e^{-i \arg P_{2m}} \, \left[\frac{1 - \cos \left[(\mathbf{P_{2m} + P_{n}}) \, \gamma\right]}{\mathbf{P_{2m} + P_{n}}} + \frac{1 - \cos \left[(\mathbf{P_{2m} - P_{n}}) \, \gamma\right]}{\mathbf{P_{2m} - P_{n}}} \right] \, . \end{split}$$

The above values of the B equation are various input parameters or functions of input parameters.

Work is continuing on this job. The program written is now being put through various production runs for Mr. Robert Mailloux who is taking over for Mr. Hans Steyskal.

We then combine the scattering matrix data produced from this (the "junction" program) with some data of the initiator to arrive at the reflected fields for the "junction" in the presence of a phased array.

A program was developed to perform this and the results were given to the investigator.

ROCKET EXHAUST PLUME STUDY

Initiator : R. E. Good LKC

Problem No.: 4683
Project No.: ILIR

The definition of high altitude rocket exhaust plumes has been developed by numerous investigators and published in various sources. It remains to solve numerically the formulation given by Hill and Jarvinen. The definition of the plume shape will be used in the determination of missile thrust.

The problem, then, is to solve numerically the following equations:

$$\begin{split} &\mathrm{I}(\theta,\phi) = \theta \, \exp \, (-\mathrm{A}^2 \widetilde{\mathrm{B}}^2) \, \sin \, \widetilde{\theta} \, \cos \, (\widetilde{\theta} - \phi) \, \, \mathrm{d}\widetilde{\theta} \\ &\beta = 1 - \cos \, (\theta + \alpha) \quad , \qquad \mathrm{A} = \pi - \left(\frac{1}{2}\right) \! \left(1 + \frac{\mathrm{T}}{\mathrm{D}}\right) \\ &\mathrm{L} = \mathrm{A} \! \left[1 + (\gamma_\mathrm{j} - 1) \, \frac{\mathrm{M}_\mathrm{e}^2}{2}\right]^{1/2} \, \left[2(\mathrm{Q}_\mathrm{j} - 1) \, \pi^3 \mathrm{M}_\mathrm{e}^2\right]^{-1/2} \, \left[1 + \frac{1}{\gamma_\mathrm{j} \mathrm{M}_\mathrm{e}^2}\right]^{-1} \\ &\mathrm{F} = \left[\mathrm{r}^2 \! \left(\frac{1}{2} \, \frac{\gamma_\mathrm{w} + 3}{\gamma_\mathrm{w} + 1} \, \sin^2 \phi + \frac{1}{\gamma_\mathrm{w} \mathrm{M}_\mathrm{w}^2}\right) - \mathrm{L} \, \exp \, (-\mathrm{A}^2 \mathrm{B}^2) \, \sin^2 \, (\theta - \phi)\right] \sin \theta \\ &\mathrm{R}_\mathrm{c} = \frac{\mathrm{r} \mathrm{I} \mathrm{L}}{\mathrm{F}} \quad . \end{split}$$

The inputs are D/T, M_e , Y_j , Y_{∞} , M_{∞} , and α . The plume shape is derived using the definition of the radius of curvature in Cartesian coordinates. The local slope of the contact surface, $\tan \varphi$, yields the first derivative. The radius of curvature, when solved by difference method, yields the change in slope:

$$\ddot{y} = \frac{(1 + \dot{y}^2)^{3/2}}{R_c}$$
.

By knowing φ initially, R_c is computed. From R_c, \ddot{Y} is determined. This permits definition of φ to start the next integration step.

The program was developed and the results presented to the investigator.

INTERPRETATIONS OF SPECTROSCOPIC DATA

Initiator : J. Manson

Problem No.: 4715

Project No. : 6688

This problem is one of explaining experimental data from a spectroscope in a rocket. Photon counts should increase at or near known laboratory spectral lines, but can vary in intensity; be contaminated by other lines nearby; suffer from general background noise; change due to noise bursts, mechanical difficulties over parts of a scan, or even variations of the transfer function of the aperture during the flight; or any combination of the above.

Since the problem involved human judgments about graphical data, it became a prime candidate for solution via interactive graphics. A program was written which plots the experimental points on a CRT screen. The user then inserts spectral lines, and is allowed to vary their intensity, shift their wavelength, and add or subtract lines thru keyboard instructions. A subroutine containing the equations of the transfer function of the spectroscope then plots the effects of this simulated data against the background of the actual data. When the user is satisfied with the goodness of fit, cards are punched out containing the wavelength and intensity of the lines as derived from this particular rocket flight. The user can then compare this flight with other flights, with laboratory experiments, or with the results of other workers in the field.

STUDY OF VARIATIONAL PRINCIPLES IN APPROXIMATIONS OF MOLECULAR CHARACTERISTICS

Initiator : K. Yoshino.

Problem No.: 4718
Project No.: 8627

This problem is involved with the study of some of the characteristics of various molecules as they change from one energy level to another as examined from a spectroscopic discipline. Since a good deal of perturbation is involved the analysis involved deals with the basic variational principles to best achieve approximations of the molecular characteristics. What is ultimately desired is the evaluation of a particular parameter, H (see below), which minimizes the perturbation in the energy changes so that calculation of molecular constants which represent certain natural elements at various energy levels may be accurately determined.

A computer program was produced to aid in determining those constants which establish at what energy state the molecules under consideration attain. The results of the approximation analysis were then compared to experimental spectroscopic data.

The analysis involved is basically the application of a linear "least squares" routine which employs variational principles, i.e., a bracketing type search performed on a particular parameter which minimizes the standard deviation of observed data to calculated data.

For each value of this variational parameter a "least squares" fit is done and a standard deviation is calculated for that particular value of the parameter so that eventually that particular value of the variational parameter for which the standard deviation is minimized is then taken to be that value which renders the least amount of perturbation.

The following is the mathematical sequence involved which describes the pertinent spectroscopic relationships required to achieve the least amount of perturbation as various energy levels are achieved:

1)
$$T_1(x) = A_1 + B_1 x - n_1 x^2$$

2)
$$T_2(x) = A_2 + B_2 x - D_2 x^2$$

3)
$$x = J(J + 1)$$
 J's are integers

4)
$$W_1(x) = (T_1(x) + T_2(x))/2 \pm (1/2) \sqrt{\delta^2 + 4H^2} + \text{when } \delta > 0$$

5)
$$W_2(x) = (T_1(x) + T_2(x))/2 \pm (1/2) \sqrt{\delta^2 + 4H^2} + \text{when } \delta < 0$$

6)
$$\delta = T_1 - T_2$$

7)
$$\delta^2 = (W_1^* - W_2^*)^2 - 4H^2$$

8)
$$T_1^*(x) = (W_1^* + W_2^*)/2 \pm \delta/2$$

9)
$$T_2^*(x) = (W_1^* + W_2^*)/2 \pm \delta/2$$

- (a) Find $\delta(J)$'s by Eq. (7) for $0 \le H \le 100$.
- (b) Find T₁(x) and T₂(x) by Eq. (8) and Eq. (9). Calculate constants A, B, and D in Eq. (1) and Eq. (2) using values of T₁(x) and T₂(x) obtained in (a).
- (c) Calculate the standard deviation of $T_1(x)$ and $T_2(x)$.
- (d) Back to (a) and repeat the steps to find that H by which the standard deviation is minimum.
- (e) Calculate $T_1(x)$ by Eq. (1), $T_2(x)$ by Eq. (2), and then calculate $W_1(x)$ by Eq. (4) and $W_2(x)$ by Eq. (5) using the value of H which minimizes the standard deviation.

Given data: $W_1^*(x)$, $W_2^*(x)$, D_1 , and D_2 .

RADIO ANTENNA PROGRAM CONVERSION

Initiator : Maj. A. Martinez

Problem No.: 4719
Project No.: 5635

The work to be done consisted of converting a large numerical analysis program for radio antennas to run on the CDC 6600.

The initiator supplied two versions of the program; one was set up to run on an IBM 360/65; the other supposedly could be run on the CDC 6600, and the hope was to reduce its core requirements and increase its efficiency.

The CDC version turned out to be in the wrong format and have irretrievable errors in the character set.

The IBM version was treated to remove syntactical errors and remove incompatibilities between the machines. It then became obvious that it would be easier to work on the CDC version, line-by-line.

Hundreds of corrections were made. Despite tremendous core memory requirements, a few simple cases were run.

In the final analysis, the initiator was supplied with an item-by-item list of why the original tape could not have been as advertised, what coding was known bad, and what was suspect.

In spite of a large amount of effort, no final program was able to be submitted to the SUYA library.

MODEL FOR THE REFRACTIVE INDEX OF STRATOSPHERIC AEROSOLS

Initiator : E.P. Shettle.

Problem No.: 4731 Project No.: 7621

<u>PURPOSE</u>: To develop an analytic expression for the refractive index of the stratospheric aerosol. This permits a more compact storage of the available data and provides an accurate extrapolation to wavelengths for which data is not available. The refractive indices as a function of wavelength will later be used to determine other optical properties of model stratospheres. The stratospheric aerosol is predominately a 75% sulfuric acid solution.

<u>DESCRIPTION:</u> (1) Do a least squares fit of given data for the real and imaginary parts (n and k, respectively) of 75% sulfuric acid solution versus frequency (ν) to the following analytic expressions:

$$k(\nu) = \sum_{j=1}^{N} \frac{B_{j} \gamma_{j} \nu}{\left(\nu_{j}^{2} - \nu^{2}\right)^{2} + \gamma_{j}^{2} \nu^{2}}$$
(1a)

$$\mathbf{n}(\nu) = \left[1 + k^{2}(\nu) + \sum_{j=1}^{N} \frac{A_{j}(\nu_{j}^{2} - \nu^{2})}{(\nu_{j}^{2} - \nu^{2})^{2} + \gamma_{j}^{2} \nu^{2}}\right]^{1/2}, \quad (1b)$$

where the A_j , B_j , γ_j , and ν_j (j = 1,..., N) are parameters whose values were to be determined by the least squares optimization.

For approximate values of the parameters, the following considerations were used:

- the ν_i fell at the peaks of $k(\nu)$
- the γ_j are the width of the peak or the distance between the corresponding turning points of $n(\nu)$
- $B_j \simeq \gamma_j \nu_j k(\nu_j)$
- $A_j \simeq 2n(\nu_j) B_j$

This leads to the following approximate values for the parameters: (j = 1, ..., 7).

i	μį	γi	<u>A</u>	B _j
1	450	70	38,000	10,500
2	580	70	60,000	25,000
3	900	50	81,000	22,000
4	1,050	70	170,000	50,000
5	1,160	200	450,000	150,000
6	1,720	210	225,000	80,000
7	2,880	800	900,000	350,000

These values were used as a starting point for a least squares iteration.

The optimization was achieved using subroutine ZXMARQ which minimizes the sum of squares of functions using a modified Marquardt algorithm. The program was first used on the real and imaginary parts separately in order to generate good initial guesses for the coefficients. These were then used as inputs to the full blown model. In all, 29 coefficients were used for the fit; 8 A_j 's and 7 each of B_j , γ_j , and ν_j .

(2) After finding the correct parameter values, calcomp plots were made comparing the fitted analytic values of n and k with the experimental data versus both frequency and wavelength.

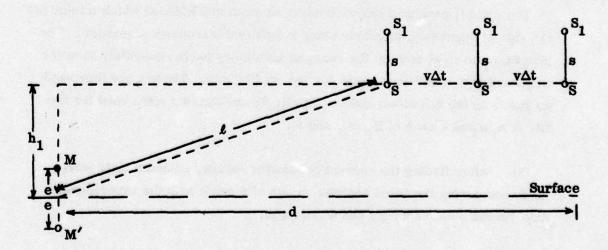
PHASE DERIVED NAVIGATION

Initiator : U. Lammers.

Problem No.: 4733
Project No.: 8682

The problem requires evaluation of a navigation system, to be used as an aircraft independent landing monitor (ILM) under multipath interference conditions. For simplicity, a two-dimensional configuration with a single image source is assumed. The type of smoothing to be used on the phase angle velocity of the received signals will be studied. Another study area involves the effects of this smoothing on the overall system accuracy.

The figure illustrates a case where a CW signal transmitted by M is received by two antennas, S and S_1 , which are spaced at a distance s and which are in linear motion. After a time interval Δt or $2\Delta t$ the antenna system moves from the right position to the center and left positions, respectively.



We call $k \cdot i_1$ the total accumulated phase shift measured at S, when S is moving from the right to the center position and $k \cdot \delta_1$ the difference in total accumulated phase between S and S₁ along the same path.

Correspondingly, quantities $k \cdot i_2$ and $k \cdot \delta_2$ are measured when moving S and S₁ from the center to the left position. Here, k is $2\pi/\lambda$ with λ the transmitted wavelength. If λ , s, Δt , i_1 , i_2 , δ_1 , and δ_2 are known the other parameters can be computed

$$\begin{split} & \ell = \frac{\delta_1 i_1 (i_1 + i_2)}{\delta_2 i_2 - \delta_1 i_1} \\ & h_1 - e = \frac{\delta_1 \delta_2 i_1 i_2 (\delta_1 + \delta_2) (i_1 + i_2)}{S(\delta_2 i_1 - \delta_1 i_1)^2} \\ & v = \frac{1}{t} \sqrt{\ell (i_2 - i_1) + 0.5(i_1 + i_2)^2 - i_1^2} . \end{split}$$

Multipath interference on this system is simulated by an image source M' of amplitude R. With signals

$$\vec{V}_S = e^{jk\overline{MS}} + Re^{jk\overline{M'S}}$$
 and $\vec{V}_{S_1} = e^{jk\overline{MS}_1} + Re^{jk\overline{M'S}_1}$

arriving at antennas S and S1 the phase angular velocities of the signals are

$$\label{eq:phi} \mathrm{d}\phi/\mathrm{d}t = \frac{\mathrm{Re}(V) \cdot \mathrm{d} \ \mathrm{Im}(V)/\mathrm{d}t - \mathrm{Im}(V) \cdot \mathrm{d} \ \mathrm{Re}(V)/\mathrm{d}t}{\mathrm{Re}^2(V) + \mathrm{Im}^2(V)} \ ,$$

where Re(V) and Im(V) represent the real and imaginary part of the \vec{v}_S , respectively, \vec{v}_S .

Quantities i_1 , i_2 , δ_1 , and δ_2 are computed through numerical integration of $d\phi/dt$. Various types of smoothing of $d\phi/dt$ under a given multipath situation are evaluated by the effect that this smoothing has on the accuracy of the output values h_1 - e, ℓ , and v. The distance ℓ is large compared with s. In this case rays arriving at S and S_1 may be considered to be parallel.

Convergence problems which have been observed are believed to be due to the basic assumption of parallel rays. Here, the cases of no multipath and perfect reflectivity (i.e., perfect symmetry) do not create a problem. However, when partial reflection is allowed the assumption of parallel rays did introduce an instability in the altitude estimate.

WITHDRAWAL WEIGHTING SYNTHESIS

Initiator : A. Slobodnick

Problem No.: 4759

Project No. : 634B-01-99

We are concerned here with the generation of time functions for withdrawal weighting. That is, we desire the overall transfer function given by D(f), where D(f) is realized by cascading two filters $H_{\underline{W}}(f)$ and $H_{\underline{A}}(f)$. Thus,

$$D(f) = H_A(f) H_w(f)$$
.

Now, $H_{W}(f)$ is fixed and specified. Therefore, we must realize $H_{A}(f)$, where $H_{A}(f)$ is given by

$$H_{A}(f) = \frac{D(f)}{H_{\mathbf{w}}(f)}.$$

Now, D(f) is to be an ideal bandpass filter, that is,

D(f) = 1 within the given band = 0 otherwise.

Therefore, we are attempting to realize

$$H_A(f) = \frac{1}{H_w(f)}$$
 within the bandwidth
= 0 otherwise .

We approximate $H_A(f)$ by a non-recursive digital filter with a frequency response given by

$$H_A(t) = a_0 + 2 \sum_{n=1}^{N} a_n \cos 2\pi f n$$
.

Now, we developed a program to determine the a_n 's to yield a minimax fit to $H_A(f)$.

The results of the design were presented to the investigator. The results were considered to be good and thus, the program was reformated into the form desired by the investigator. The final program was given to the investigator for his use.

MEASUREMENT OF AMBIENT ELECTRIC FIELD

Initiator: M. Smiddy.

Problem No.: 4764

Project No. : 8617

The measurement of ambient electric fields on two rockets is part of a large AFCRL program involving chemical release and mass-spectrometer measurements.

The processing involved can be divided into three phases where one phase must be completed before commencement of the next.

- I. Digitizing of: 1) Rocket trajectory data.
 - 2) Rocket attitude data.
 - 3) Experiment data ΔV .

All input data will be on magnetic tape and computer (CDC 6600) output tapes are required.

II. Trajectory and attitude data to be processed to give probe position and attitude data as a function of time-from-launch.

One vehicle (A10.302-1) has three-axis fluxgate magnetometers for attitude. The second vehicle (A10.403-3) has magnetometers and a gyro for attitude acquisition — this flight has also a mass-spectrometer aboard who will also require attitude processing.

III a. Two dipole E-field data reduced to give three spatial components E_x , E_y , and E_z also components along and perpendicular to geomagnetic field B. This is performed in a way which is dependent

dent on the vehicle motion but is performed by subtracting the Lorenze field produced by vehicle motion from the measured field at a time t (above 80 km altitude),

$$\vec{E} \cdot \vec{R} = \frac{V}{|R|} - (\vec{v} \times \vec{B}) \cdot \vec{R} ,$$

where E = ambient electric field vector

R = dipole position vector

|R| = length of dipole

V = voltage differences measured

v = vehicle velocity vector

 \vec{B} = geomagnetic field vector.

Other diagnostic information is also computed such as: a function which shows the magnitude of the magnetic field connection area between the vehicle and the dipole sensors; the velocity vector location in relation to the dipole axes.

III b. The A10.302-1 rocket has also a spherical electrostatic analyzer for measuring electron density and temperature. The equations and mode of processing this data will be made available as required (the method is similar to data processed on ISIS-I and INJUN-V satellites).

CONTOUR OF EARTH DEFORMATION DUE TO CHEMICAL EXPLOSION

Initiator : M. Settle.

Problem No.: 4774
Project No.: 7639

Recent research on deformation in granular earth materials (e.g., soils and sands) produced by chemical explosions is being conducted within the Terrestrial Sciences Laboratory. Field tests conducted nearby at Ft. Devens have been designed to specifically measure in situ ground strengths both before and after the detonation of a chemical explosive. Ground strength measurements are recorded as continuous 'profiles' on a penetrometer device which probes to depths up to 20 inches along a single profile. The purpose of this research is to ultimately delineate the extent and geometry of the zone of permanent deformation surrounding the crater produced by such explosions.

Two programs were written to do the above described job. The first program generated the probe curve equations of ground "strength" values for a given set of probes and combines deep input probes. It consists in producing mathematical equations which accurately describe ground "strength" measurements recorded as continuous "profile" on a penetrometer device which probes into the ground.

The second program uses the output of the first to generate a contour plot of ground "strength" values within given horizontal and vertical distances from the center of explosion. The contour plot is drawn from a set of given values produced from the input probe equations.

LAMB WAVE VELOCITY DISPERSION

Initiator : T.L. Szabo

Problem No.: 4787 Project No.: 5635

Lamb waves are accoustic waves that propagate in plates at a velocity determined by its frequency and the thickness, density, and elastic constants of the plate. Calculations of the velocity of the first-order symmetric and anti-symmetric Lamb modes are required for nondestructive evaluation of stressed plates.

For a given type of elastic solid the longitudinal (c_{ℓ}) and bulk (c_{t}) wave velocities are known. The velocities of the first-order symmetric (s_{0}) and anti-symmetric (s_{0}) modes are to be calculated and plotted as a function of the running parameter 2fh, which is the frequency (f), thickness (2h) product of the plate in which these Lamb waves propagate.

The following equations govern the velocity:

If
$$u = \frac{C_+^2}{C_-^2}$$
 and $v = \frac{C_+^2}{C_1^2}$

the first-order symmetric mode equation is

$$\frac{\tan (1-u)^{1/2} \frac{\pi}{C_{+}} (2fh)}{\tan (v-u)^{1/2} \frac{\pi}{C_{-}} (2fh)} = -\frac{4u(1-u)^{1/2} (v-u)^{1/2}}{(2u-1)^{2}}$$

and the first-order antisymmetric mode equation is

$$\frac{\tan (1-u)^{1/2} \frac{\pi}{C_{+}} (2fh)}{\tan (v-u)^{1/2} \frac{\pi}{C_{+}} (2fh)} = -\frac{(2u-1)^{2}}{4u(1-u)^{1/2} (v-u)^{1/2}}.$$

These equations are solved for c using the root finding routine ZREAL2.

The program has been run for a variety of materials and parameters as requested by the initiator.

ACOUSTIC WAVE BEAMSHAPING

Initiator : T. L. Szabo.

Problem No.: 4788

Project No.: 5635

This problem deals with acoustic wave beamshaping for non-destructive testing. (Ultrasonic non-destructive evaluation of defects is complicated by changes in the beam pattern caused by diffraction.)

18 versions of programs were written. 10 of these are in the process of being submitted to the SUYA library.

These computer programs deal with aspects of simulating various waveshapes as they propagate along a material. They progress to one which can analyze any arbitrary shape at the launching transducer, and culminate in one which reconstruct what the signal must have looked like at the launching transducer, from the way it looked when picked up further along the material.

The goals originally envisioned in the statement of work have more than been accomplished. Any of the various encouraging possibilities opened up by these programs will have to be re-initiated as a separate problem in the future.

A CALCULATION OF FOURIER HARMONICS

Initiator : A. Cole

Problem No.: 4793

Project No.: 8624

This problem is involved in calculating A_0 , A_1 , A_2 , φ_1 , and φ_2 in the following equation:

$$y(x) = A_0 + A_1 \sin (x + \varphi_1) + A_2 \sin (2x + \varphi_2)$$

where x = iZ, Z = 360/period

i = 0, 3, 6, 9, 12, 15, 18, 21

 $A_0 = mean$

A₁ = amplitude of the first harmonic

A₂ = amplitude of the second harmonic .

A table of values of y's are to be supplied by the initiator.

A Fourier analysis computer program was developed to successfully produce the desired harmonics. The results of this effort were used in the overall patterns of a meteorological study.

INTEGRAL COMPUTATIONS USING GAUSS-MEHLER QUADRATURE

Initiator : D. Freeman

Problem No.: 4808 Project No.: 6687

<u>PROBLEM DESCRIPTION</u> Experimental values are given for the discrete vibrational energies G(v) with $v=0,1,...,v_{max}$ and for the rotational constants B(v) with $v=0,1,...,v_{max}$. We wish to compute the integrals:

$$f_v = 4.1057886M^{-1/2} \int_{v_{min}}^{v} [G(v) - G(v')]^{-1/2} dv'$$
 (1)

and

$$g_v = 0.24355857M^{1/2} \int_{v_{min}}^{v} B(v')[G(v) - G(v')]^{-1/2} dv'$$
 (2)

using Gauss-Mehler quadrature, as described by Tellinguisen. This technique is fast and avoids the singularity at the upper limits of integration. The reduced mass M of the oscillator and the value of v_{max} are given. The lower limit of integration is

$$v_{\min} = -\frac{1}{2} - \delta \tag{3}$$

with

$$\delta = (2x)^{-1}[(w^2 + 4xY)^{1/2} - w] \tag{4}$$

and

$$Y = -\frac{1}{4} \left[x - B \left(\frac{\alpha w}{6B^2} + 1 \right)^2 \right] . \qquad (5)$$

The values of G(v) and B(v) at $v = v_{min}$ are, if $\delta \neq 0$,

$$G(v_{\min}) = -Y \tag{6}$$

and

$$B(v_{min}) = B + \alpha \delta + \gamma \delta^2 . (7)$$

In Eqs. (4)-(7), the vibrational parameters w and x, and the rotational constants B, α , and γ are given. If $\delta = 0$, set

$$v_{\min} = -\frac{1}{2}$$
, $G(v_{\min}) = Y = 0$, $B(v_{\min}) = B$.

The program provides the option of constructing G(v') and B(v') in Eqs.

- (1) and (2) in either one or both of the following ways:
- (a) G(v') and B(v') are constructed as piecewise analytic functions of v' by performing cubic Hermite interpolation between consecutive experimental values, and the required derivatives at each such point are formed artificially by a finite difference approximation.²
- (b) G(v') and B(v') are represented by the power series

$$G(v') = \sum_{i=1}^{6} C_{vi} \left(v' + \frac{1}{2}\right)^{i}$$
 (8)

$$B(v') = \sum_{i=1}^{6} C_{ri} \left(v' + \frac{1}{2}\right)^{i-1}$$
 (9)

in which the coefficients are supplied as input.

It is known that G(v) increases monotonically with v and usually has a negative second derivative and that B(v) decreases monotonically with v and usually has a negative first derivative. The coefficients in Eqs. (8) and (9) decrease rapidly in magnitude as i increases.

OUTPUT A title such as "RKR curve for the ground state of CO"

Reduced mass M = · · · ·

Vibrational parameters:

a listing of the coefficients in Eq. (8) if used Rational constants:

a listing of the coefficients in Eq. (9) if used A tabulation of the following quantities:

v, B(v), G(v) + Y, $2f_v$, $20g_v$, R_v (outer), R_v (inner) for the values $v = v_{min}$, $n \in with n = 0, 1, 2, ..., v_{max} / \epsilon$. A step size ϵ is given, normally in the range 0.25 - 5.0. The quantities R_v (outer) and R_v (inner) are defined by

$$R_{v}(\text{outer}) = \left(f_{v}^{2} + \frac{f_{v}}{g_{v}}\right)^{1/2} + f_{v} \quad \text{and} \quad R_{v}(\text{inner}) = \left(f_{v}^{2} + \frac{f_{v}}{g_{v}}\right)^{1/2} - f_{v}.$$

Also, given as output are the quantities: δ , Y, B(v_{min}), R(v_{min}). The quantity R(v_{min}) is defined as

$$R(v_{min}) = 4.1057886M^{-1/2}[B(v_{min})]^{-1/2}$$
.

SAMPLE PROBLEM Data and results for the ground state of CO are contained in the references.

REFERENCES (attached)

- 1. J. Tellinguisen, Computer Phys. Commun. 6, 221 (1974);
 - J. Tellinguisen, J. Mol. Spectrosc. 44, 194 (1972).
- 2. P. Tsipouras and R. V. Cormier, AFCRL-TR-73-0400 (1973).
- 3. A.W. Mantz, et al., J. Mol. Spectrosc. 39, 180 (1971).

COMPUTER MODIFICATION USED IN THE CALCULATION OF RADIAL AND TANGENTIAL DISPLACEMENTS OF THE ELASTODYNAMIC FIELD

Initiator

P. Michaels

Problem No. :

4813

Project No. :

7639

This problem deals with the modification of a computer program, ELAS, which calculates the radial and tangential displacements of the Elastodynamic field radiated by an impulsive force acting normal to a line in the surface of a semi-infinite medium.

This problem is a continuation of a problem that is described in detail in AFCRL-68-0481. The total problem is concerned with the detection and analysis of underground seismic waves.

The determination of stress components of a cylindrical S-wave and P-wave propagated in a pre-stressed medium has been determined. The investigation and analysis has been completed in the determination of stress components which involve the following simulated stresses:

- a stress field around a hole in an otherwise unaxial compression field (1),
- a pure shear field around a field (2),
- a pure tension field around a hole (3),
- and any additive combination of 1 thru 3.

Richard W. Doherty, Joseph F. Russell, and Rose M. Ring, Scientific Research in the Form of Numerical Analysis and Data Analysis, AFCRL-68-0481, Bedford, Mass., p. 30.

Another force was introduced into the pre-stressed medium. This new force was a dipole radiation. Hence, a program was written to determine stress components for dipole radiation. These components were determined from the following equations:

$$\sigma r = -AdCp \left(\frac{\sin \theta}{\sqrt{r}}\right)^2 G\left(t - \frac{r}{Cp}\right) - ApCp \frac{1}{\sqrt{r}} F\left(t - \frac{r}{Cp}\right)$$

 $\sigma\theta = \delta\sigma r$

$$\tau r\theta = AdCs \frac{\cos 2\theta}{\sqrt{r}} G_1 \left(t - \frac{r}{Cs}\right)$$
,

where: If $0 \le [t - (r/Cp)] \le then,$

$$F\left(t - \frac{r}{Cp}\right) = \sin\frac{2\pi}{T}\left(t - \frac{r}{Cp}\right)$$

otherwise, F[t - (r/Cp)] = 0.

If $[t - (r/Cp)] \ge 0$, then

$$G\left(t - \frac{r}{Cp}\right) = \exp\left[-\frac{1}{t_0^2}\left(t - \frac{r}{Cp} - t_0\right)^2\right]$$

otherwise, G[t - (r/Cp)] = 0.

If $[t - (r/Cs)] \ge 0$, then

$$G\left(t - \frac{r}{Cs}\right) = \exp\left[-\frac{1}{t_0^2}\left(t - \frac{r}{Cs} - t_0\right)^2\right]$$

otherwise, G[t - (r/Cs)] = 0.

The range of the parameters is as follows:

$$0^{\circ} \le \theta \le 90^{\circ}$$
 $\Delta \theta = 10^{\circ}$
1.0 $\le r \le 2.0$ $\Delta(r) = .1$
2.0 $< r \le 90$ $\Delta(r) = 1.0$
Ad = .5, Ap = 1.0, T = 1.0, and $t_0 = .4$, $\delta = .4$

The required modifications were made to the computer program, ELAS, mentioned above and was subsequently submitted to the Computer User's Library at AFGL, Hanscom Field.

TAPE EVALUATION

Initiator : L. Logan

Problem No.: 4815

Project No.: 7630

The problem consisted of evaluating a tape produced by a specialized balloon recording system, pending acceptance of the hardware by the Air Force.

Several programs were written, and various tape dumps were made at Mitre. Unfortunately, a total of 6 tapes were finally supplied, none of them being in the advertised hardware format.

Thus, the original goal of evaluating the consistency of the data became subordinate to getting any proper data at all.

The latest program was handed over to the initiator, for him to incorporate in any future testing efforts. No program was submitted to the SUYA library since there never was any proper data supplied.

POTENTIAL BETWEEN TWO RARE GAS ATOMS

Initiator : D. Freeman

Problem No.: 4817 Project No.: 6687

PROBLEM DESCRIPTION The distribution of the eigenvalues E(v) of a potential V(R) is given by (Ref. 1)

$$\frac{dv}{dE(v)} = A \int_{R_1(v)}^{R_2(v)} [E(v) - V(R)]^{-1/2} dR , \qquad (1)$$

in which A is a known constant and E(v) is the eigenvalue of the discrete level v which has inner and outer turning points $R_1(v)$ and $R_2(v)$, respectively. A simple approximation to be long-range potential between two rare gas atoms is

$$V(R) = D - C_R R^{-6}$$
, (2)

in which D is the unknown dissociation limit and C_6 is a known constant related to the outer turning point by the expression

$$E(v) = D - C_6 R_2^{-6} . (3)$$

Reference (1) shows that the substitution of Eqs. (2) and (3) into Eq. (1) leads to

$$\frac{dv}{dE(v)} = AC_6^{-1/2}R_2^4 \int_1^{R_2/R_1} y^{-2}(y^6 - 1)^{-1/2} dy , \qquad (4)$$

in which $y = R_2 R^{-1}$ and the integral is known in the limit $R_2/R_1 \rightarrow \infty$ in terms of gamma functions. Equations (3) and (4) then yield

$$\frac{dE(v)}{dv} = K_6[D - E(v)]^{2/3}$$
, (5)

in which K_6 is a collection of known constants. If $v = v_D$ is defined as the vibrational index (generally nonintegral) at the dissociation limit, $E(v_D) = D$, the integrated form of Eq. (5) is

$$D - E(v) = -\left[\frac{K}{3}(v_D - v)\right]^3$$
 (6)

The problem is to find analogous, preferably in analytical form, of Eqs. (4), (5), and (6) when, instead of using the pair of Eqs. (2) and (3), we use one of the more accurate pairs

$$V(R) = D - C_{c}R^{-6}(1 + \beta R^{-2})$$
 (7a)

$$E(v) = D - C_6 R_2^{-6} (1 + \beta R_2^{-2})$$
 (7b)

$$V(R) = D - C_6 R^{-6} \exp(\beta R^{-2})$$
 (8a)

$$E(R) = D - C_6 R_2^{-6} \exp(\beta R_2^{-2})$$
 (8b)

$$V(R) = D - C_{\alpha}R^{-6}(1 - \beta R^{-2})^{-1}$$
 (9a)

$$E(R) = D - C_g R_2^{-6} (1 - \beta R_2^{-2})^{-1}$$
, (9b)

in which βR^{-2} and βR_2^{-2} are small (<0.2) compared to unity. We require the problem to be solved only for any one of Eqs. (7), (8), or (9), not necessarily for all three.

POLYNOMIAL FIT A polynomial approximation of the form

$$V(R) = D - cR^{-6}(1 + \beta R^{-2} + \gamma R^{-4})$$

$$E(v) = D - cR_{2}^{-6}(1 + \beta R_{2}^{-2} + \gamma R_{2}^{-4}) , \qquad (10)$$

is adopted for integral (1) by which it becomes a function of β and γ . A bivariate polynomial is fit to the computed values of dv/dE(v).

REFERENCES

- 1. R.J. Le Roy and P.B. Bernsten, J. Chem. Phy. 52, 3869 (1970).
- 2. S. M. Kirschner and J. K. Watson, J. Mol. Spectroscopy, 47, 2346 (1973).

NUMERICAL MAPPING OF IONOSPHERIC PARAMETERS ON A GLOBAL BASIS

Initiator : J. Kotelly

Problem No.: 4825

Project No.: 7663

The problem is to investigate methods of numerical mapping ionospheric parameters on a global basis; specifically, this involves developing the capability to plot values of FOF 2 as a function of geomagnetic latitude for a constant local mean time.

This problem was acquired only a few weeks before the end of the period covered by this report, and will be carried into a future one.

Several computer programs were written for the set of data presented, but they only proved that the data had many transcription errors.

Several computer programs were written for a second set of data, but progress must be halted until the cards designating the observing stations arrive at AFGL.

TAPE REFORMATTING

Initiator : E. Robinson

Problem No.: 4826 Project No.: 6690

Project No. : 6690

This problem involves reformatting SAMTEC TRAE radar tracking data from IBM 7094 binary tape into the standard SUYA CDC 6600 radar tape format.

A program was written to perform the above, and to produce time plots of azimuth, altitude, and range as well.

Continued minor changes have been made, mostly to augment the control the user has over what gets plotted, since in practice it seems the radar track spurious objects before and after the desired flights.

INVERSION OF LIMB AIRGLOW MEASUREMENTS

Initiator : R. A. Van Tassel.

Problem No.: 4828
Project No.: 6688

This analysis provides support for an optical mission on the Defense Meteorological Satellite System (DMSS). The objectives are:

- Computation of theoretical optical volume emission rates as a function of altitude;
- 2. Computation of the simulated output of the DMCS sensor system; and
- Development of an inversion algorithm to infer ionospheric parameters from DMSS data.

PART I. Theoretical Optical Volume Emission Rates

The computation of theoretical optical volume emission rates as a function of altitude will be computed for two different mechanisms: 1) radiative recombination, and 2) electron impact excitation.

For radiative recombination, we will use the formula

$$F(z) = \alpha n(z)^2 ,$$

where F(z) is the volume emission rate, α is the rate coefficient, and n(z) is the number of electrons/cm³, given by the relation

$$N(z) = n_{max} \exp \frac{1}{2} \left[1 - \frac{z - z_{max}}{SH_e} - \exp \left(- \frac{z - z_{max}}{SH_e} \right) \right].$$

In this relation, S is a shape factor and H is the electron scale height.

Initial computations may use values as follows:

$$\alpha$$
 = 8 × 10⁻¹³ cm³ sec⁻¹,
 n_{max} = 10⁵ electrons cm⁻³,
 z_{max} = 250 km, and
 SH_e = 50 km.

The required range of F(z) is from 200 to 500 km in increments of 1 km. The units of F(z) are photons cm⁻³.

In order to compute theoretical emission rates resulting from electron impact, we use the formula,

$$F(z) = n_0(z) \int \sigma(\epsilon) n_e(z, e) d\epsilon ,$$

where $n_0(z)$ is the number density of atomic oxygen in cm⁻³, $\sigma(\epsilon)$ is the cross section for electron-impact excitation of the $^5\mathrm{S}^0$ state in atomic oxygen as a function of electron energy, and $n_{\mathrm{e}}(z,\epsilon)$ is the electron energy distribution function. The range and increments are again 200 to 500 km in 1 km increments.

The function $n_0(z)$ is available from a model atmosphere which is already stored in the computer. An experimental determination of $\sigma(\epsilon)$ is shown in Figure 1. The electron energy distribution is being calculated by another program in this work unit. Paul Tsipouras (SUYA) is familiar with this program.

PART II. Simulated Satellite Output

The computation of the simulated output of the DMSS sensor system involves computing the column emission rate by integrating along lines-of-sight or ray

paths. The effects of absorption along the ray path is included. The expression for the column emission rate 4%I(h) is given by

$$4\pi I(h) = 4\pi I_{\perp}(h) + 4\pi I_{\perp}(h)$$
,

where

$$4\pi I_{\pm}(h) = \int_{h}^{\infty} F(z) e^{-\sigma_{\lambda} N_{\pm}(h, z)} \left(\frac{dx}{dz}\right) dz ,$$

and

$$\left(\frac{dx}{dz}\right) = \frac{(R_e + z)}{A(h, z)}$$

with A(H, z) given by

$$A(h, z) = \sqrt{z^2 - h^2 + 2R_e(z - h)}$$
,

where h identifies the ray path by its tangent altitude and R_e is the radius of the earth.

Initially we will assume an isothermal atmosphere above 200 km, so that we may express $N_{\pm}(h,z)$, the number of absorbers along the path from the emitting point to the sensor located mathematically at infinity, by

$$\begin{split} N_{+}(h,z) &= n_{0} \Biggl(-A(h,z) e^{-z/H} + \left(\frac{1}{H} \right) \int_{z}^{\infty} A(h,\xi) e^{-\xi/H} d\xi \Biggr) \\ N_{-}(h,z) &= n_{0} \Biggl(-A(h,z) e^{-z/H} + \left(\frac{1}{H} \right) \int_{h}^{\infty} A(h,\xi) e^{-\xi/H} d\xi \Biggr) \\ &+ \left(\frac{1}{H} \right) \int_{z}^{h} A(h,\xi) e^{-\xi/H} d\xi \Biggr) , \end{split}$$

where H is the scale height for molecular oxygen.

These results should be compared with results using the expressions

$$N_{+}(h, z) = \int_{z}^{\infty} n(\xi) \frac{(R_{e} + \xi)}{A(h, \xi)} d\xi$$

and

$$N_{-}(h,z) = \int_{h}^{\infty} n(\xi) \frac{(R_{e} + \xi)}{A(h,\xi)} d\xi + \int_{z}^{h} n(\xi) \frac{(R_{e} + \xi)}{A(h,\xi)} d\xi ,$$

where $n(\xi)$ is the O_2 number density from a model atmosphere which is stored in the computer.

PART III. The Development of an Inversion Algorithm

The first two parts of this problem were concerned with calculating theoretical values for F(z) and then $4\pi I(h)$ from a relationship of the form

$$4\pi I(h) = \int F(z) k(h, z) dz .$$

The third part of this problem is the inverse of the second part, i.e., to infer F(z) given several observations for $4\pi I(h)$. The general approach to this kind of retrieval problem has been to assume an initial form for F(z) and to compare calculated values of $4\pi I(h)$ with observed values. Iteration is continued until the desired degree of accuracy between calculated and observed values of $4\pi I(h)$ is obtained.

COLLIMATOR PROGRAM CONVERSION

Initiator : R. Fredrickson.

Problem No.: 4852

Project No. : 5621

This job was essentially a conversion job. A Fortran program written previously to run on another computer was converted to run on the CDC 6600 computer here. This program gives the results of a Monte Carlo calculation of the energy spectrum and angular distribution of a gamma radiation emitted by a collimated Cobalt-60 source. The program was developed flexible enough to give results for a wide variety of geometric situations of source container and collimator.

In making this conversion a Fortran utility routine had to be used to replace an existing assembly language subroutine which was untransferrable.

The program was run with several test cases varying certain input parameters to obtain several sets of output. After close examination of this output the initiator was assured of the correctness of the program.

SIGNAL ANALYSIS OF ROCKET DATA

Initiator : T. Conley

Problem No.: 4854

Project No. : 7660

This problem is to develop a computerized system, including appropriate computer programs and operator instructions, to digitally filter (smooth) unwanted noise from rocket measured radiometer and photometer data (in digital form), correct data for rocket aspect, and digitally differentiate smoothed data to obtain volume emission rates. Current ICECAP rocket radiometer measured data is contaminated by noise induced by the telemetry recording and digitization processes and which leads to erroneous volume emission rates when differentiated,

Considerable data exists at OPR (approximately 10 rocket flights) which need analysis by this technique.

Sample data was copied from tapes and programs were developed to perform initial processing on the data. Specifically, a noise filter and differentiation filter programs were written and used on the data. These test results were in excellent agreement with known results. The net noise suppression obtained [noise filter minus differentiation] was greater than 60 db.

Thus, development of a complete system is underway as outlined below.

Work on this problem will be continued under another contract.

Processing Procedure for Emission Rate Determination

- I. Establish data file.
 - Edit data (replace calibration and noise "spike" points in data) using optimal fitting.
 - Convert to Brightness Unit (Rα).
 - Plot resulting Ra data vs. time.
 - Produce and plot FFT of data.
 - Van Rhijn Aspect Correction ($R_0 = R\alpha/\sqrt{\alpha}$).
 - Plot resulting Ra data vs. time.
 - Produce and plot FFT of data.
- II. Design a noise filter and process data through the filter
 (possibly separate filters for precession and wideband noise).
 - · Plot filtered data (vs. time).
- III. Differentiate output of noise filter (using a differentiation filter).
 - Plot resulting output (vs. time).
 - Convert to desired variables (emission rate vs. altitude) and produce plot.

WAVELENGTH PEAK STUDY

Initiator : T. Conley

Problem No.: 4855

Project No.: 7670

This problem is to develop a computerized system to smooth noise contaminated spectral features in rocket measured CVF data (ICECAP data) in order to accurately specify wavelength of peak emission features and determine line widths. This technique is required to analyze existing data (approximately 5 rocket flights).

A noise filter is being developed for this data. However, no data processing has been begun to date. Also, techniques for "optimal" estimation of peak locations are being studied. In particular, the possible use of full band differentiations (with variance estimates) is being studied.

Work on this problem will be continued under another contract.

STATISTICAL ANALYSIS OF GAS MEASUREMENT DATA

Initiator : C.C. Gallagher

Problem No.: 4861 Project No.: 6687

The problem is to develop statistical techniques to identify gas measurements from column and spectrometer tests. Using calibration and test runs procedures for specifying an identification procedure is to be developed including probability measures of the uncertainties.

A program has been developed to calculate the "statistics" of the calibration and test runs and provide student t tests for most probable compounds. Sample data will be used to evaluate the approach.

Work on this problem will be continued under another contract.

ACKNOWLEDGEMENTS

The support offered during the extent of this contract was coordinated and evaluated by the contract monitor, Dr. Paul Tsipouras (SUA). We offer a simple thanks for his valuable help.

Thanks also to Mrs. Rita de Clercq Zubli, technical typist to the secretarial staff, who made this report possible.